

Abstract Submitted  
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**Charge-Transport Parameters in Molecular Organic Semiconductors.** VEACESLAV COROPCEANU, PAVEL PARAMONOV, ROEL S. SÁNCHEZ-CARRERA, DEMETRIO A. DA SILVA FILHO , JEAN-LUC BREDAS, Georgia Institute of Technology — In this contribution we will discuss the present state-of-the-art in the derivation of electronic and electron-phonon coupling constants in organic semiconductors from quantum-chemical calculations. We will reveal some of the shortcomings of the current models used to depict organic semiconductors and also the paths to be followed to achieve significant improvements. The contributions of both intra-molecular and inter-molecular vibrations to the electron-phonon interaction will be discussed in detail. Our results show that for an adequate description of the charge transport in organic semiconductors both local and non-local electron-phonon mechanisms should be taken into account. In the case of oligoacene crystals several phonon modes that contribute most strongly to the modulation of the transfer integrals were found to display large nonlinear electron-phonon couplings.

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